SYMMETRIES IN NUCLEI AND MOLECULES

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ABSTRACT

Recent progress in two different fronts is reported. First, the concept of bisection of a harmonic oscillator or hydrogen atom, used in the past in establishing the connection between U(3) and O(4), is generalized into multisection (trisection, tetrasection, etc). It is then shown that all symmetries of the N-dimensional anisotropic harmonic oscillator with rational ratios of frequencies (RHO), some of which are underlying the structure of superdeformed and hyperdeformed nuclei, can be obtained from the U(N) symmetry of the corresponding isotropic oscillator with an appropriate combination of multisections. Furthermore, it is seen that bisections of the N-dimensional hydrogen atom, which possesses an O(N+1) symmetry, lead to the U(N) symmetry, so that further multisections of the hydrogen atom lead to the symmetries of the N-dim RHO. The opposite is in general not true, i.e. multisections of U(N) do not lead to O(N+1) symmetries, the only exception being the occurence of O(4) after the bisection of U(3). Second, it is shown that there is evidence that the recently observed in superdeformed nuclear bands $\Delta I = 4$ bifurcation is also occuring in rotational bands of diatomic molecules. In addition there is evidence that a $\Delta I = 8$ bifurcation, of the same order of magnitude as the $\Delta I = 4$ one, is observed in superdeformed nuclear bands and rotational bands of diatomic molecules.

1. Introduction

In this paper two different topics will be presented. The first (sections 2–9) is related to the symmetries of the anisotropic harmonic oscillator with rational ratios of frequencies. The second (sections 10–14) is related to a novel staggering effect observed recently in superdeformed nuclear bands.

2. Multisections of the harmonic oscillator

Anisotropic harmonic oscillators with rational ratios of frequencies (RHOs) [1-7] are of current interest in several branches of physics. Their symmetries form the basis for the understanding [8-12] of the occurence of superdeformed and hyperdeformed

nuclear shapes [13,14] at very high angular momenta. In addition, they have been recently connected [15,16] to the underlying geometrical structure in the Bloch–Brink α-cluster model [17]. They are also becoming of interest for the interpretation of the observed shell structure in atomic clusters [18], especially after the realization that large deformations can occur in such systems [19]. An interesting problem is to what extend the various symmetries of the RHOs, occuring for different frequency ratios, are related to other known symmetries. A well-known example is the case of the 3-dimensional RHO with frequency ratios 2:2:1, which is known to possess the O(4) symmetry [20].

In this study we show how the symmetries of the N-dim RHO can be obtained from the U(N) symmetry of the corresponding isotropic harmonic oscillator (HO) by appropriate symmetry operations, namely multisections, which are generalizations of the concept of bisection, introduced in [20]. It will furthermore be shown that these symmetries can also be obtained from the O(N+1) symmetry of the N-dim hydrogen atom, since a bisection leads from O(N+1) to U(N), so that further multisections lead to RHO symmetries. However, despite the fact that the N-dim RHO symmetries can be obtained from the O(N+1) symmetry by appropriate multisections, they are not orthogonal symmetries themselves (with the exception of 2:2:1 mentioned above).

In section 3 of this paper the Hamiltonian of the N-dim RHO is given. Multisections of the 3-dim and the N-dim harmonic oscillator are defined and used in obtaining the symmetries of the various RHOs in sections 4 and 5 respectively. The N-dim hydrogen atom is briefly described in section 6. A similar procedure is followed in sections 7 and 8 for the 3-dim and the N-dim hydrogen atom, while section 9 contains a summary of the present results and implications for further work.

3. The anisotropic harmonic oscillator with rational ratios of frequencies (RHO)

The Hamiltonian of the N-dim RHO reads

$$H = \frac{1}{2} \sum_{k=1}^{N} \left(p_k^2 + \frac{x_k^2}{m_k^2} \right),$$
(1)

where m_i are natural numbers prime to each other. The energy eigenvalues are given by

$$E = \sum_{k=1}^{N} \frac{1}{m_k} \left(n_k + \frac{1}{2} \right),$$
(2)

where n_k is the number of quanta in the k-th direction.

4. Multisections of the 3-dimensional oscillator

Let us consider the completely symmetric irreps of U(3), $[N00]$, the dimensions

of which are given by

$$d(N) = \frac{(N+1)(N+2)}{2}, \qquad N = 0, 1, 2, \ldots \tag{3}$$

Using the Cartesian notation (n_x, n_y, n_z) for the U(3) states, as in [20], one can easily see that a **bisection** of the 1:1:1 RHO states (having degeneracies 1, 3, 6, 10, 15, 21, ..., given by eq. (3)) distinguishing states with $\mathrm{mod}(n_z, 2) = 0$ and states with $\mathrm{mod}(n_z, 2) = 1$, results it two interleaving 2:2:1 sets of levels, having degeneracies 1, 2, 4, 6, 9, 12, 16, 20, ...

By analogy, a **trisection** can be made by distinguishing states with $\mathrm{mod}(n_z, 3) = 0$ or $\mathrm{mod}(n_z, 3) = 1$ or $\mathrm{mod}(n_z, 3) = 2$. The degeneracies obtained are 1, 2, 3, 5, 7, 9, 12, 15, 18, ..., which correspond to the 3:3:1 RHO. Therefore a trisection of the 1:1:1 HO results in three interleaving sets of 3:3:1 RHO states.

Similarly a **tetrasection** is defined by selecting states with $\mathrm{mod}(n_z, 4) = 0$, or 1, or 2, or 3. The degeneracies obtained are 1, 2, 3, 4, 6, 8, 10, 12, 15, 18, ..., which characterize the 4:4:1 RHO. Therefore a tetrasection of the 1:1:1 HO leads to four interleaving sets of 4:4:1 RHO states.

In general, an *n-section* of the 1:1:1 HO is obtained by separating states with $mod(n_z, n) =$0, or 1, or 2, ..., or $n - 1$. In this case n interleaving sets of the n:n:1 RHO states, which corresponds to an oblate shape, are obtained. It is clear that n-sections using n_x or n_y instead of n_z lead to the same conclusions.

One can consider successively more than one bisections, trisections, etc. Let us consider more than one bisections first.

Getting the results of the $\mathrm{mod}(n_z, 2) = 0$ bisection of the HO and applying a $\mathrm{mod}(n_y, 2) =$0 bisection on them we obtain the degeneracy pattern 1, 1, 3, 3, 6, 6, 10, 10, i.e. "two copies" of the 1:1:1 degeneracies, which corresponds to the 2:1:1 RHO. The same result is obtained for any combination of two bisections along two differerent axes.

Bisecting the 1:1:1 HO for a third time, along the x-axis this time by using $\mathrm{mod}(n_x, 2) =$0, one obtains the degeneracy pattern 1, 3, 6, 10, ..., i.e. that of the original 1:1:1 HO.

Furthermore one can easily see that:

i) Two trisections along different axes lead to degeneracies 1, 1, 1, 3, 3, 3, 6, 6, 6, ..., i.e. to the 3:1:1 RHO pattern ("three copies" of the 1:1:1 degeneracies).

ii) Three trisections lead to the original 1:1:1 HO degeneracy pattern.

iii) Two tetrasections lead to degeneracies 1, 1, 1, 1, 3, 3, 3, 3, 6, 6, 6, 6, ..., i.e. to the 4:1:1 RHO pattern ("four copies" of the 1:1:1 degeneracies).

iv) Three tetrasections lead back to the original 1:1:1 HO pattern.

The results obtained so far are summarized in Table 1.

In general one can see that:

i) Two n-sections (along different axes) lead to the degeneracy pattern of n:1:1, i.e. to "n copies" of the 1:1:1 degeneracies. n:1:1 corresponds to a prolate shape.

ii) Three n-sections lead back to the degeneracy pattern of the 1:1:1 HO.

Table 1

Degeneracies of various 3-dim anisotropic harmonic oscillators with rational ratios of frequencies (RHOs) obtained from the U(3) symmetry of the isotropic 3-dim harmonic oscillator (HO) by the application of various multisections. The first line corresponds to the isotropic 3-dim HO. In the rest of the lines the first column contains the appropriate multisection, while the second column contains the frequency ratios $m_1 : m_2 : m_3$ of the resulting RHO.

U(3)	1:1:1	1	3	6	10	15	21	28	36			
1 bisection	2:2:1	1	2	4	6	9	12	16	20			
1 trisection	3:3:1	1	2	3	5	7	9	12	15	18	22	26	30
1 tetrasection	4:4:1	1	2	3	4	6	8	10	12	15	18	21	24
2 bisections	1:1:2	1	1	3	3	6	6	10	10	15	15	21	21
2 trisections	1:1:3	1	1	1	3	3	3	6	6	6	10	10	10
2 tetrasections	1:1:4	1	1	1	1	3	3	3	3	6	6	6	6
3 bisections	1:1:1	1	3	6	10	15	21	28	36			
3 trisections	1:1:1	1	3	6	10	15	21	28	36			
3 tetrasection	1:1:1	1	3	6	10	15	21	28	36			

One can, of course, apply successive n-sections with different n. For example, applying $\mod(n_z, 2) = 0$, $\mod(n_y, 3) = 0$ and $\mod(n_x, 3) = 0$ one obtains the degeneracy pattern 1, 1, 2, 1, 2, 4, 2, 4, 6, ..., which corresponds to the 2:2:3 oscillator.

In general one can see that by applying a k-section, an l-section and an m-section along different axes one obtains the degeneracy pattern $(kl) : (mk) : (lm)$, where common factors appearing in all three quantities (kl), (mk), (lm) can be dropped out.

We have therefore seen that all the symmetries of the 3-dim RHO can be obtained from the U(3) symmetry of the isotropic 3-dim HO by an appropriate set of n-sections.

A special remark can be made about the 2:2:1 case. The degeneracies obtained there correspond to the dimensions of the irreps of O(4), given by

$$d(\mu_1, \mu_2) = (\mu_1 + \mu_2 + 1)(\mu_1 - \mu_2 + 1). \tag{4}$$

In particular, the degeneracies 1, 4, 9, 16, ... correspond to the integer irreps $(\mu, 0)$ with $\mu = 0, 1, 2, 3, \ldots$, while the degeneracies 2, 6, 12, 20, ... correspond to the spinor irreps $(\frac{n}{2}, \frac{1}{2})$ with $n = 1, 3, 5, 7, \ldots$. This result has been first found by Ravenhall et $al.$ [20]. It has been pointed out that O(4) is obtained by imposing a reflection condition on U(3). For example, O(4) is obtained by selecting the states with n_z=odd, a procedure which is equivalent to the insertion of an impenetrable barrier across the xy plane.

5. Multisections of the N-dimensional oscillator

The symmetry is U(N). If N is even, there is an Sp(N) subalgebra, if N is odd there is no such subalgebra.

N bisections lead back to the U(N) irreps.

N−1 bisections lead to the 2:1:1:...:1 symmetry, i.e. to "two copies" of the U(N) irreps.

N−2 bisections lead to the 2:2:1:1:...:1 symmetry, which bears certain similarities to O(N+1). The dimensions of the integer irreps are obtained correctly. The dimensions of the odd irreps differ by a factor of $2^{\nu-1}$, where $\nu = N/2$ for N even or $\nu = (N-1)/2$ for N odd. Therefore the 2:2:1:1:...:1 symmetry is not in general O(N+1).

N−3 bisections lead to the 2:2:2:1:1:...:1 degeneracies.

Two bisections lead to the 2:2:...:2:1:1 degeneracies.

One bisection leads to the 2:2:...:2:2:1 degeneracies.

Similarly

one n-section leads to the n:n:...:n:n:1 degeneracies,

two n-sections lead to the n:n:...:n:1:1 degeneracies,

N−2 n-sections lead to n:n:1:...:1:1,

N−1 n-sections lead to n:1:1:...:1:1,

N n-sections lead back to U(N).

6. The hydrogen atom

So far we have considered multisections of the N-dim harmonic oscillator. We are now going to consider multisections of the hydrogen atom (HA) in N dimensions, which is known to be characterized by the O(N+1) symmetry [21], which is also the symmetry characterizing a particle constrained to move on an (N+1)-dim hypersphere.

7. Multisections of the 3-dimensional hydrogen atom

The 3-dim hydrogen atom is known to possess the O(4) symmetry. We know that the irreps of O(4) are characterized by two labels μ_1, μ_2 and are denoted by (μ_1, μ_2), while the irreps of O(3) are characterized by one label $\mu_1' = L$ (the usual angular momentum quantum number) and are denoted by (μ_1'). When making the reduction O(4) $\supset$ O(3), μ_1' obtains all values permitted by the condition $\mu_1 \geq \mu_1' \geq \mu_2$ [22]. Furthermore, the decomposition O(3)$\supset$O(2) can be made, the irreps of O(2) characterized by the quantum number $M = L, L-1, L-2, \ldots, -(L-1), -L$.

We are going to consider the completely symmetric irreps of O(4), which are of the form $(\mu_1, 0)$. Writing down the (LM) states contained in each O(4) irrep one finds that the dimensions of the irreps are 1, 4, 9, 16, 25, ..., as expected from eq. (4), since only the integer irreps occur. As pointed out by Ravenhall et $al.$ [20], a

bisection can be effected by inserting an impenetrable barrier through the center of the hydrogen atom. Only the states with $L - M$=odd remain then.

The resulting degeneracies are again 1, 3, 6, 10, 15, 21, ..., i.e. U(3) degeneracies. Therefore a **bisection** of the 3-dim hydrogen atom, effected by choosing states with $\text{mod}(L - M, 2) = 0$ or $\text{mod}(L - M, 2) = 1$, is leading to two interleaving sets of U(3) states, having degeneracies 1, 3, 6, 10, 15, ... Choosing states with $\text{mod}(L + M, 2) = 0$ or 1 obviously leads to the same results.

The fact that by bisecting O(4) one obtains U(3) has been first pointed out by Ravenhall *et al.* [20]. Once the U(3) symmetry of the 3-dim HO is obtained, any further multisections on it will lead to RHO degeneracies, as pointed out in subsec. 2.1.

8. Multisections of the N-dimensional hydrogen atom

The N-dim hydrogen atom is characterized by the O(N+1) symmetry. Only the completely symmetric irreps of O(N+1) occur. Using the chain O(N+1) $\supset$ O(N) $\supset$ ... $\supset$ O(3) $\supset$ O(2) one can find the (LM) states contained in each O(N+1) irrep. Bisecting them using $\text{mod}(L - M, 2) = 0$ or 1 one is left with the irreps of U(N). Further multisections of the U(N) irreps lead to the appropriate symmetries of the N-dim RHO. It is therefore clear that all symmetries of the N-dim RHO can be obtained from a common parent, the O(N+1) symmetry. Thus it is not surprising that some of them (notably the 2:2:1:...:1 ones) show similarities to the corresponding O(N+1) symmetry. However, the only case in which an N-dim RHO symmetry is identical to an O(N+1) symmetry occurs for N=3, for which the 2:2:1 RHO symmetry is O(4) [20]. The rest of the RHO symmetries are not related to any orthogonal symmetries.

9. Multisections: summary

The concept of bisection of an N-dim isotropic harmonic oscillator with U(N) symmetry, introduced by Ravenhall *et al.* [20], has been generalized. Trisections, tetrasections, ..., n-sections of the N-dim isotropic harmonic oscillator have been introduced. They are shown to lead to the various symmetries of the anisotropic N-dim harmonic oscillator with rational ratios of frequencies (RHO). Furthermore, multisections of the N-dim hydrogen atom with O(N+1) symmetry have been considered. It is shown that a bisection of O(N+1) leads to U(N), so that further multisections just lead to various cases of the N-dim RHO. The opposite does not hold, i.e. multisections of U(N) do not lead to O(N+1) symmetries, the only exception being the bisection of U(3) which does lead to O(4). Even in the case of the 4-dim HO, which has the U(4) symmetry, which is isomorphic to O(6) and has an O(5) subalgebra, no multisection, or combination of multisections, leading to a RHO with O(5) symmetry can be found. We conclude therefore that the rich variety of the N-dim RHO symmetries have a common "parent", the U(N) symmetry of the N-dim isotropic harmonic oscillator or the O(N+1) symmetry of the N-dim hydrogen atom, but they are not in general related to unitary or orthogonal symmetries themselves.

Since the RHO is of current interest in relation to various physical systems (superdeformed and hyperdeformed nuclei [8-12], Bloch–Brink α-cluster model [15-17], deformed atomic clusters [18,19]), the unification of the rich variety of symmetries appearing in the RHO for different frequency ratios in a common algebraic framework is an interesting project. In [6] the 3-dim RHO degeneracies are obtained as reducible representations of U(3). It could be possible to construct an algebraic framework in which the RHO degeneracies occur as irreducible representations of an appropriate algebra. Work in this direction is in progress [23,24].

Throughout this study the properties of the completely symmetric irreps of U(N) and O(N+1) have been considered. Similar studies of completely antisymmetric irreps, or irreps with mixed symmetry, might be worth exploring.

10. Novel staggering effects in rotational bands

Rotational bands of diatomic molecules [25] and rotational bands of deformed nuclei [26] have many features in common, despite the different energy scales involved in each case. Molecular rotational bands are in general closer to the behavior of the rigid rotator than their nuclear counterparts. In the last decade much interest has been attracted by superdeformed nuclear bands [13,14,27], which are characterized by relatively high angular momenta and behavior closer to the rigid rotator limit in comparison to normal deformed nuclear bands.

A rather surprising feature has been recently discovered [28,29] in superdeformed nuclear bands: Sequences of states differing by four units of angular momentum are displaced relative to each other, the relative shift being of order of 10^{-4} of the energies separating the levels of these bands. A few theoretical proposals for the possible explanation of this $\Delta I = 4$ bifurcation, which is also called $\Delta I = 2$ staggering, have already been made [30-33].

A reasonable question is therefore whether $\Delta I = 4$ bifurcations (i.e. $\Delta I = 2$ staggering), observed in nuclear superdeformed bands as discussed in section 11, also occur in rotational spectra of diatomic molecules. We are going to show in section 12 that this is indeed the case. Bifurcations with $\Delta I = 8$ and $\Delta I = 12$ will also be discussed in section 13, while section 14 will contain a summary of the present results and discussion of further work.

11. $\Delta I = 2$ staggering in superdeformed nuclear bands

In nuclear physics the experimentally determined quantities are the γ-ray transition energies between levels differing by two units of angular momentum ($\Delta I = 2$). For these the symbol

$$E_{2,\gamma}(I) = E(I+2) - E(I) \qquad (5)$$

is used, where $E(I)$ denotes the energy of the level with angular momentum I. The deviation of the γ-ray transition energies from the rigid rotator behavior can be

measured by the quantity [29]

$$\Delta E_{2,\gamma}(I) = \frac{1}{16}(6E_{2,\gamma}(I) - 4E_{2,\gamma}(I-2) - 4E_{2,\gamma}(I+2) + E_{2,\gamma}(I-4) + E_{2,\gamma}(I+4)). \quad (6)$$

Using the rigid rotator expression $E(I) = AI(I+1)$ one can easily see that in this case $\Delta E_{2,\gamma}(I)$ vanishes. This is due to the fact that eq. (6) is the discrete approximation of the fourth derivative of the function $E_{2,\gamma}(I)$.

Several nuclear superdeformed rotational bands such as (a) to (e) for ^{149}Gd [28] and the bands (1) to (3) for ^{194}Hg [29] were analyzed. The corresponding tables are not included in this short presentation, being reserved for a forthcoming longer publication. The analysis shows that the $\Delta E_{2,\gamma}(I)$ values exhibit an anomalous staggering. It should be noted, however, that only for the band (a) of ^{149}Gd [28], the amplitude of the oscillations (see for example fig. 3 of ref [29]) is definitely outside the experimental errorbars. The following observations can be made:

i) $\Delta E_{2,\gamma}(I)$ obtains alternating positive and negative values. This is why this effect has also been called "$\Delta I = 2$ staggering".

ii) The magnitude of $\Delta E_{2,\gamma}(I)$ is of order 10^{-4}–10^{-5} of that of the γ-ray transition energies.

iii) The staggering oscillation width is an increasing function of the angular momentum I.

12. $\Delta I = 2$ staggering in rotational bands of diatomic molecules

In the case of molecules the experimentally determined quantities regard the R branch $(I \rightarrow I + 1)$ and the P branch $(I \rightarrow I - 1)$. They are related to transition energies through the equations [34]

$$E^R(I) - E^P(I) = E_{v=1}(I+1) - E_{v=1}(I-1) = DE_{2,v=1}(I-1), \quad (7)$$

$$E^R(I) - E^P(I+2) = E_{v=0}(I+2) - E_{v=0}(I) = DE_{2,v=0}(I), \quad (8)$$

where in general
$$DE_2(I) = E(I+2) - E(I), \quad (9)$$

and v is the vibrational quantum number. $\Delta I = 2$ staggering can then be estimated by using eq. (6), with $E_{2,\gamma}(I)$ replaced by $DE_2(I)$:

$$\Delta E_2(I) = \frac{1}{16}(6DE_2(I) - 4DE_2(I-2) - 4DE_2(I+2) + DE_2(I-4) + DE_2(I+4)). \quad (10)$$

It is noted, that for the sake of simplicity a normalized form of the discrete fourth derivative is used in (10) as well as in the subsequent equations : (11), (13), and (15). We have analyzed quite a few molecular rotational bands for several diatomic molecules. The detailed results are saved for a longer publications. Some of the bands revealing a staggering effect are:

i) The (1-1), $v=1$ rotational band of the $C^1\Sigma^+$–$X^1\Sigma^+$ system of YD (data from [35]).

ii) The (2-2), $v = 1$ rotational band of the $A^1\Sigma^+$–$X^1\Sigma^+$ system of YN (data from [36]).

iii) The (4-3), $v=1$ band for the molecule CS (data from [37]).

Similar results have been obtained from the other available bands of these molecules and from the $A^6\Sigma^+$–$X^6\Sigma^+$ system of CrD (data from [38]). The following comments are in place:

i) $\Delta E_2(I)$ exhibits alternating signs with increasing I, a fingerprint of $\Delta I = 2$ staggering for the $v = 1$ band, while the $v = 0$ band data do not permit a rigorous identification of the staggering effect.

ii) The magnitude of the perturbation, $\Delta E_2(I)$, is of order 10^{-3}–10^{-5} of that of the interlevel separation energy.

iii) The staggering oscillation width is not a monotonically increasing function of the angular momentum I. The irregularities in the magnitude of $\Delta E_2(I)$ might indicate the presence of subsequent bandcrossings [39]. It is known that the bandcrossing effect is seeing only when the interaction between the two bands which cross each other is relatively weak [40]. Therefore only the levels neighboring the crossing are affected by the interaction. From eq. (10) it is then clear that perturbing an energy level results in perturbing 5 consequent values of $\Delta E_2(I)$. In view of this, case i) looks very much like depicting two subsequent bandcrossings. Cases ii) and iii), however, do not immediately accept such an interpretation. Bandcrossing has been recently suggested as a possible source of the $\Delta I = 4$ bifurcation in nuclei [41,42]. Certainly more work is needed in this direction.

iv) The staggering effect is more prominent in the case of even angular momentum data than in the case of odd angular momentum data.

13. $\Delta I = 4$ and $\Delta I = 6$ staggering in nuclei and molecules

One might further wonder if bifurcations with $\Delta I > 4$ can also occur. In the nuclear case, the existence of $\Delta I = 4$ staggering can be checked by using the quantity

$$\Delta E_{4,\gamma}(I) = \frac{1}{16}(6E_{4,\gamma}(I) - 4E_{4,\gamma}(I-4) - 4E_{4,\gamma}(I+4) + E_{4,\gamma}(I-8) + E_{4,\gamma}(I+8)), \quad (11)$$

where

$$E_{4,\gamma}(I) = E(I+4) - E(I). \quad (12)$$

Results for several superdeformed nuclear bands have been calculated. A good example is provided by the $\Delta I = 8$ bifurcation for the superdeformed band (a) of ^{149}Gd [28]. Note that no angular momentum assignments can be made, since they are still uncertain. The following remarks apply:

i) $\Delta E_{4,\gamma}(I)$ acquires alternating signs with increasing I, indicating the existence of a $\Delta I = 8$ bifurcation.

ii) The order of magnitude of the $\Delta I = 4$ staggering is the same as that of the $\Delta I = 2$ staggering.

In the case of diatomic molecules one can search for $\Delta I = 4$ staggering by using

the quantity

$$\Delta E_4(I) = \frac{1}{16}(6DE_4(I) - 4DE_4(I-4) - 4DE_4(I+4) + DE_4(I-8) + DE_4(I+8)), \quad (13)$$

where

$$DE_4(I) = E(I+4) - E(I). \quad (14)$$

In our study we have analyzed the larger known bands of the molecule CS, i.e. the bands (1-0) $v = 1$, (2-1) $v = 0$, (4-3) $v = 0$, (2-1) $v = 0$ [37]. The results for the rotational bands of the $A^6\Sigma^+$–$X^6\Sigma^+$ system of CrD (data from [38]), the $C^1\Sigma^+$–$X^1\Sigma^+$ system of YD (data from [35]), and the $A^1\Sigma^+$–$X^1\Sigma^+$ system of YN (data from [36]) were also considered. For these molecules experimental data of long enough bands exist, permitting the calculations. A good example is provided by the $\Delta I = 4$ staggering ($\Delta I = 8$ bifurcation) for the (1-1), $v = 1$ band of the $C^1\Sigma^+$–$X^1\Sigma^+$ system of the molecule YD. The following comments can be made:
i) Alternating signs of $\Delta E_4(I)$, a fingerprint of $\Delta I = 8$ bifurcation, are observed.
ii) The magnitude of the $\Delta I = 4$ staggering appears to be the same as that of the $\Delta I = 2$ staggering.
$\Delta I = 12$ bifurcation i.e. $\Delta I = 6$ staggering can be searched for through use of the quantity

$$\Delta E_6(I) = \frac{1}{16}(6DE_6(I) - 4DE_6(I-6) - 4DE_6(I+6) + DE_6(I-12) + DE_6(I+12)), \quad (15)$$

where

$$DE_6(I) = E(I+6) - E(I). \quad (16)$$

Calculations have been carried out for a few cases of rotational bands of CS (data from [37]), and for the $B^1\Sigma_u^+$–$X^1\Sigma_g^+$ system of $^{63}Cu^{65}Cu$ (data from [43]), in which bands long enough for such a calculation are known. These results look like being in favor of the existence of $\Delta I = 6$ staggering of the same order of magnitude as $\Delta I = 4$ and $\Delta I = 2$ staggering, but they are not enough for drawing any final conclusions.

14. Novel staggering effects: summary

The observation of $\Delta I = 2$ and $\Delta I = 4$ staggering in rotational spectra of diatomic molecules offers a corroboration of the existence of the same effect in nuclei, since the experimental techniques used in each case are quite different, so that the occurrence of the same systematic errors in both cases is improbable. Furthermore, the energy scales involved in nuclei and molecules are very different (the separation of energy levels in molecules is of the order of 10^{-2}eV, while in nuclei of the order of 10^5eV), but the staggering effects are in both cases of the same order of magnitude relative to the separation of the energy levels, indicating that the same basic mechanism, possibly related to some perturbations of given symmetry, might be responsible for these effects in both cases.

In conclusion, we have shown that:

i) $\Delta I = 2$ staggering, first observed in superdeformed nuclear bands [28,29], occurs as well in rotational bands of diatomic molecules.

ii) In all cases the magnitude of the $\Delta I = 2$ staggering is 10^{-3}–10^{-5} of that of the separation of the energy levels.

iii) Furthermore $\Delta I = 4$ staggering appears to be present both in superdeformed nuclear bands as well as in rotational bands of diatomic molecules, its order of magnitude being the same as that of the $\Delta I = 2$ staggering in the same physical system.

iv) In most cases the magnitude of the staggering does not show a simple dependence on angular momentum. In several cases one sees about 5 points deviating very much for the smooth rotational behavior, then several points much closer to the pure rotational behavior, then again about 5 points deviating very much from the smooth rotational behavior, and so on. Such a picture raises suspicions for the presence of bandcrossings at the points at which the large deviations occur [41,42].

Concerning the theoretical explanation of the $\Delta I = 2$ staggering effect, some proposals in the nuclear physics framework already exist [30–33]. However, one cannot draw any firm conclusions up to now. In view of the present results, further efforts, in investigating other molecular and nuclear data, are necessary.

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16. References

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